Efficient Encoding of Quantum States for Hamiltonian Simulation of (2+1)-dimensional U(1) Lattice Gauge Theory with Finite Temperature

Reita Maeno/ International Center for Elementary Particle Physics (ICEPP), University of Tokyo

A work in progress with Koji Terashi, Lento Nagano, Sanmay Ganguly, Yasuyuki Okumura, Yutaro Iiyama

Background

- Nonperturbative numerical simulation of gauge theory
  ▶ Lattice Gauge Theory (LGT)

- Conventional calculation: Monte Carlo method

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, \mathcal{O} e^{-S_E(\phi)} \overset{\text{Regularization}}{\blacktriangleright} \sum_{\{\phi_i\}} \mathcal{O}_i \frac{e^{-S_E(\phi_i)}}{Z}$$

Regard this as probability
▶ Do Monte Carlo

- In some systems, $e^{-S_E(\phi_i)}/Z$ becomes complex

▶ Hard to compute precisely ⋯ Sign problem

▶ Need to consider alternative calculation method

Example of sign problem:
- Real-time dynamics
- Finite density system
- Topological term

Hamiltonian formulated LGT

Hamiltonian formulated LGT

- Compute Hilbert space **directly**

  $$|\psi(0)\rangle \xrightarrow{\ e^{-iHt}\ } |\psi(t)\rangle$$

  ✓ Free from sign problem

  $\longrightarrow$ time

  ✗ Increase computational resources exponentially for system sizes...?

Hamiltonian formulated LGT

Hamiltonian formulated LGT

- Compute Hilbert space **directly**

  $$|\psi(0)\rangle \xrightarrow{e^{-iHt}} |\psi(t)\rangle$$
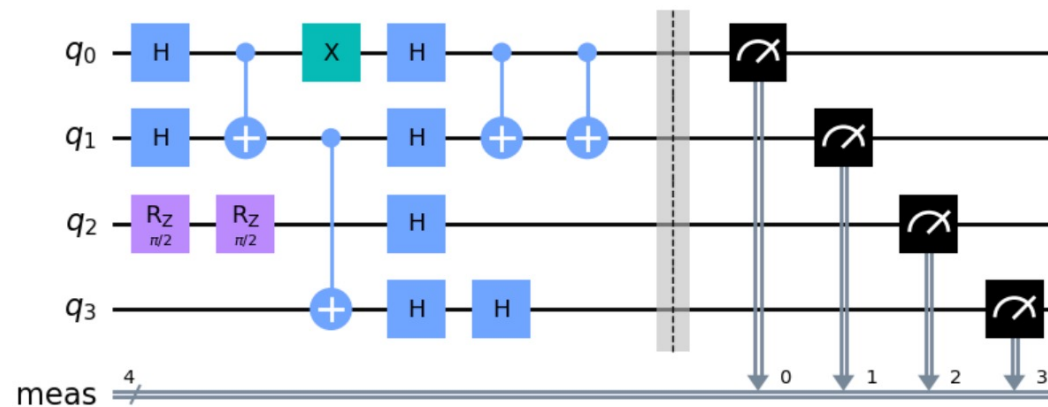
  time

  ✓ Free from sign problem

  ✗ Increase computational resources exponentially for system sizes...?

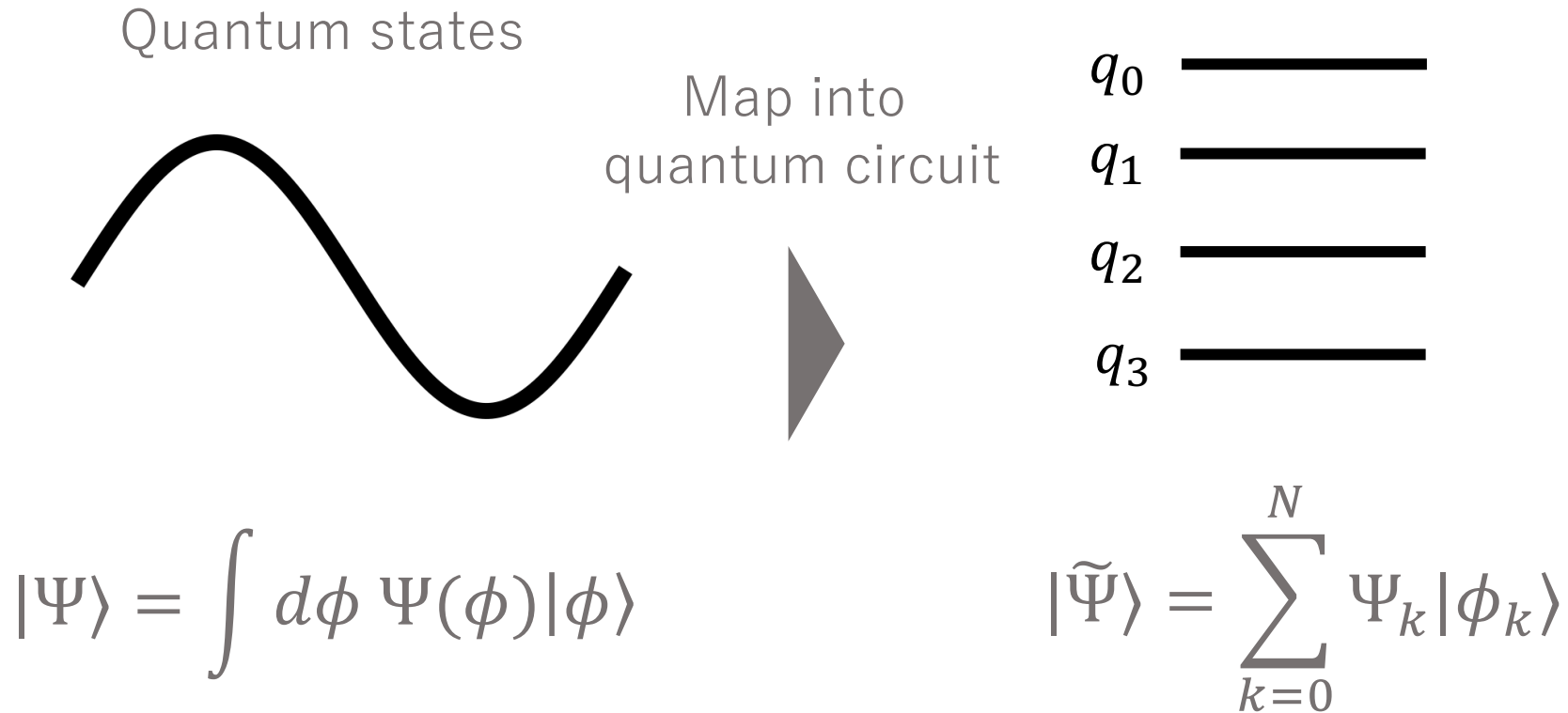 > ▶ Quantum computers have potential to overcome!
  > (※Tensor network also has)

Towards quantum computation of gauge fields

- Quantum states of gauge fields have infinite D.O.F.
- ▶ Truncation is necessary to implement on classical/quantum computer

Quantum states

Map into
quantum circuit

q_0 ▬▬▬

q_1 ▬▬▬

q_2 ▬▬▬

q_3 ▬▬▬

$$|\Psi\rangle = \int d\phi\, \Psi(\phi)|\phi\rangle$$

$$|\widetilde{\Psi}\rangle = \sum_{k=0}^{N} \Psi_k |\phi_k\rangle$$

Previous works on formulation

- Important to choose bases with large contribution
- Important to reduce the size of Hilbert space by utilizing Gauss' law

Example of Previous works

- R/B formulation [J. F Haase et al., 2021]
  - Canonical Commutation Relation (CCR) method [C. W. Bauer, D. M. Grabowska, 2023]
- Kogut-Susskind [J. Kogut, L. Susskind, 1975][T. Byrnes, Y, Yamamoto, 2006]
- Loop-String-Hadron [I. Raychowdhury, J. R. Stryker, 2020]
- Quantum link model [U. J. Wiese, 2013]
- Quantum group [T. V. Zache et al., 2023]
- Orbifolds [A. J Buser et al., 2021]
- Light-Front [Kreshchuk et al., 2020]
- Fuzzy fields [Alexandru et al., 2024]
- Spin-dual [Mathur et al., 2016]

Previous works on formulation

- Important to choose bases with large contribution
- Important to reduce the size of Hilbert space by utilizing Gauss' law

Example of Previous works

- R/B formulation [J. F Haase et al., 2021]

  - Canonical Commutation Relation (CCR) method [C. W. Bauer, D. M. Grabowska, 2023]

  Utilize this method later

- Kogut-Susskind [J. Kogut, L. Susskind, 1975][T. Byrnes, Y, Yamamoto, 2006]

- Loop-String-Hadron [I. Raychowdhury, J. R. Stryker, 2020]

- Quantum link model [U. J. Wiese, 2013]

- Quantum group [T. V. Zache et al., 2023]

- Orbifolds [A. J Buser et al., 2021]

- Light-Front [Kreshchuk et al., 2020]

- Fuzzy fields [Alexandru et al., 2024]

- Spin-dual [Mathur et al., 2016]

Optimization of digitization of quantum states

Canonical Commutation Relation (CCR) method [C. W. Bauer, D. M. Grabowska, 2023]

- One of the way to optimize quantum states with magnetic basis
  - ▶ The paper focuses on optimization of **low-lying states**

    in pure (non-)compact (2+1)-dimensional U(1) LGT

Optimization of digitization of quantum states

Canonical Commutation Relation (CCR) method [C. W. Bauer, D. M. Grabowska, 2023]

■ One of the way to optimize quantum states with magnetic basis

▶ The paper focuses on optimization of **low-lying states**

in pure (non-)compact (2+1)-dimensional U(1) LGT

▶ What about **excited states**? i.e. finite temperature $T \neq 0$

※ For example, we need to consider thermal properties to simulate finite density systems

Optimization of digitization of quantum states

Canonical Commutation Relation (CCR) method [C. W. Bauer, D. M. Grabowska, 2023]

- One of the way to optimize quantum states with magnetic basis

  ▶ The paper focuses on optimization of **low-lying states**

    in pure (non-)compact (2+1)-dimensional U(1) LGT

  ▶ What about **excited states**? i.e. finite temperature $T \neq 0$

  ※ For example, we need to consider thermal properties to simulate finite density systems

- In this work, we focus on efficient basis choice under $T \neq 0$

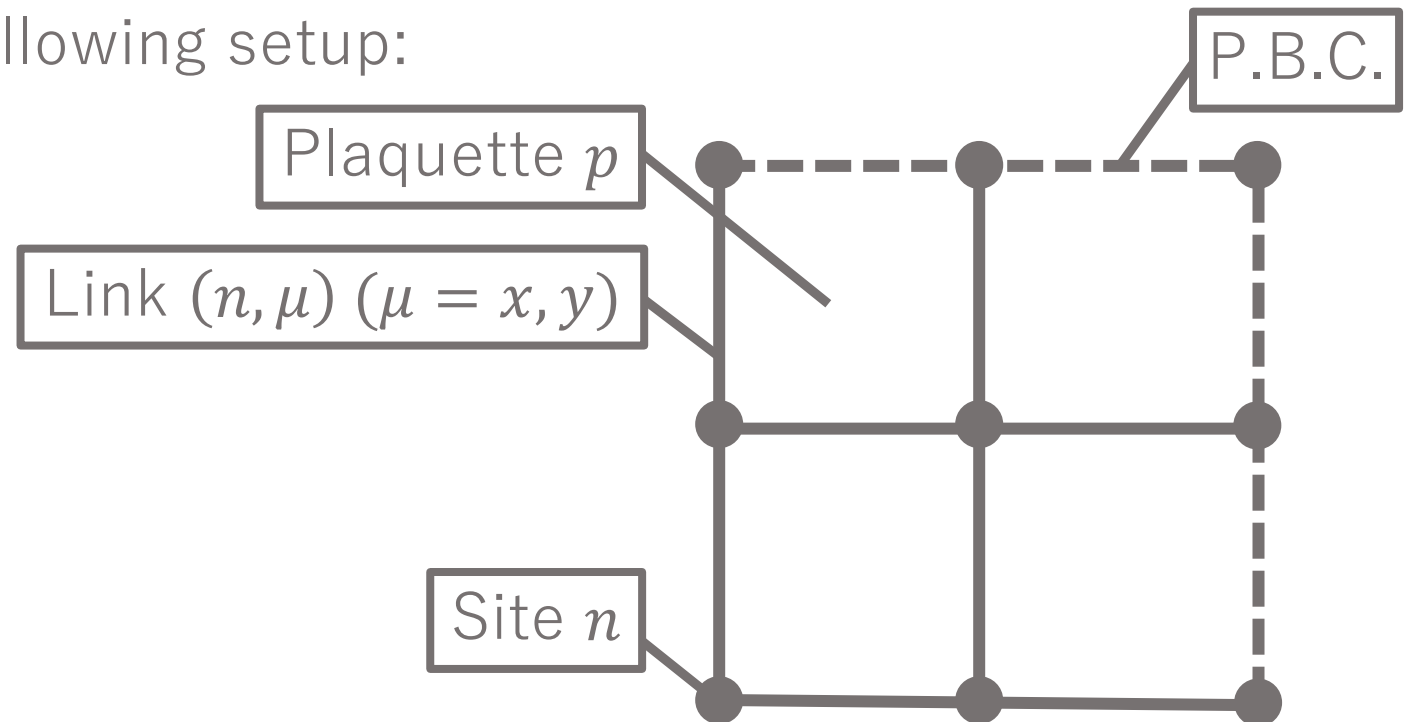|	**Pure compact U(1)**	**Compact U(1) w/. fermion**
Low-lying states	Previous work	This work
Excited states	This work	This work

Contents
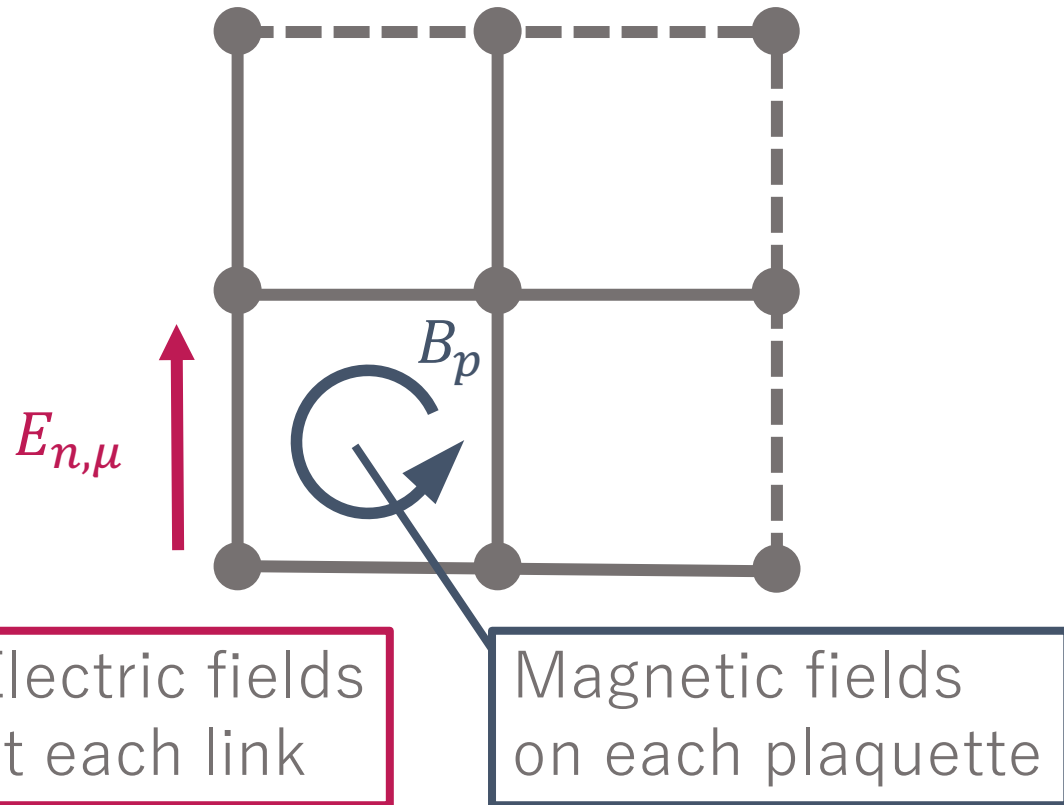
- Introduction

- Results
  Ⅰ. Pure compact U(1)
  Ⅱ. Compact U(1) including matter

Setup

- We consider two models :
  - Pure compact U(1) LGT
  - Compact U(1) LGT including fermion

- For simplicity, we consider following setup:
  - Four lattice points
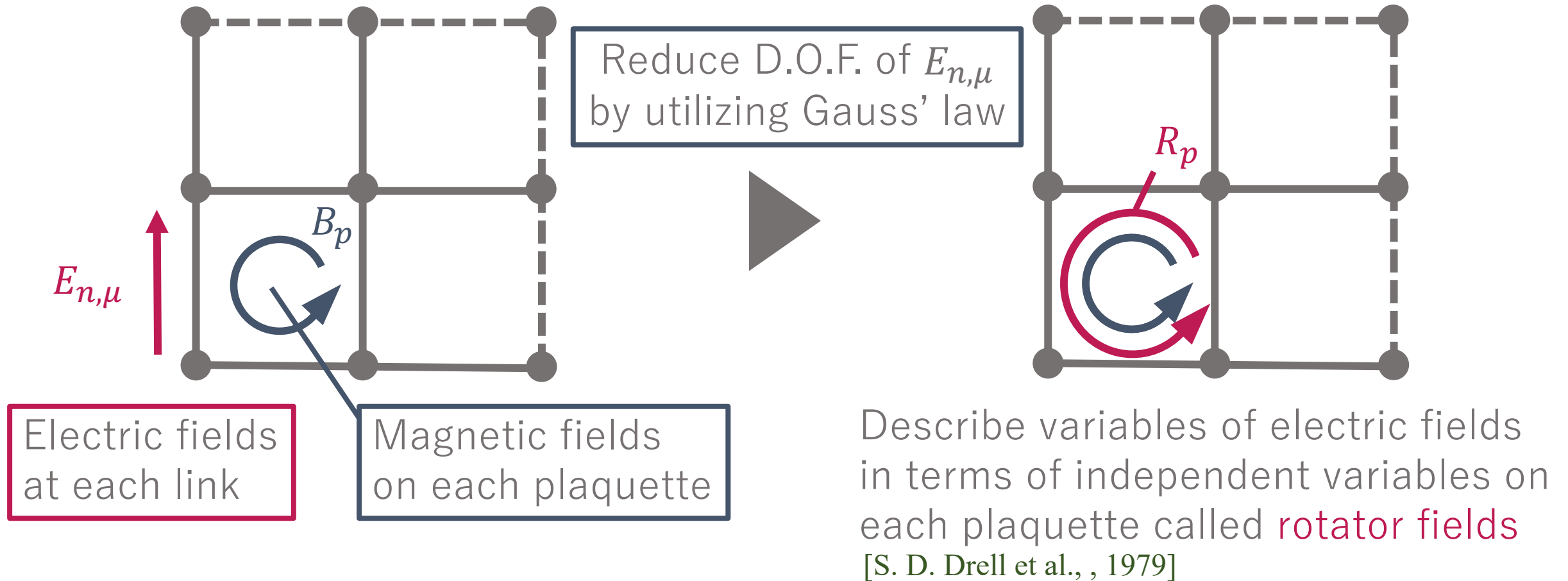 - Periodic Boundary condition (P.B.C.)

P.B.C.

Plaquette p

Link (n, μ) $(\mu = x, y)$

Site n

Pure compact U(1) LGT

$E_{n,\mu}$

B_p

Electric fields
at each link

Magnetic fields
on each plaquette

Pure compact U(1) LGT

Reduce D.O.F. of $E_{n,\mu}$
by utilizing Gauss' law

B_p

$E_{n,\mu}$

R_p

Electric fields
at each link

Magnetic fields
on each plaquette

Describe variables of electric fields
in terms of independent variables on
each plaquette called rotator fields
[S. D. Drell et al., , 1979]

Pure compact U(1) LGT

- The resulting Hamiltonian:

$$H = H_E^{(\text{pure})} + H_B$$

$$aH_E^{(\text{pure})} = 2g^2[R_1^2 + R_2^2 + R_3^2 - R_1(R_2 + R_3)]$$

$$aH_B = -\frac{1}{g^2}[\cos(B_1) + \cos(B_2) + \cos(B_3)$$
$$+\cos(B_1 + B_2 + B_3)]$$

R_4/B_4 can be removed by P.B.C.
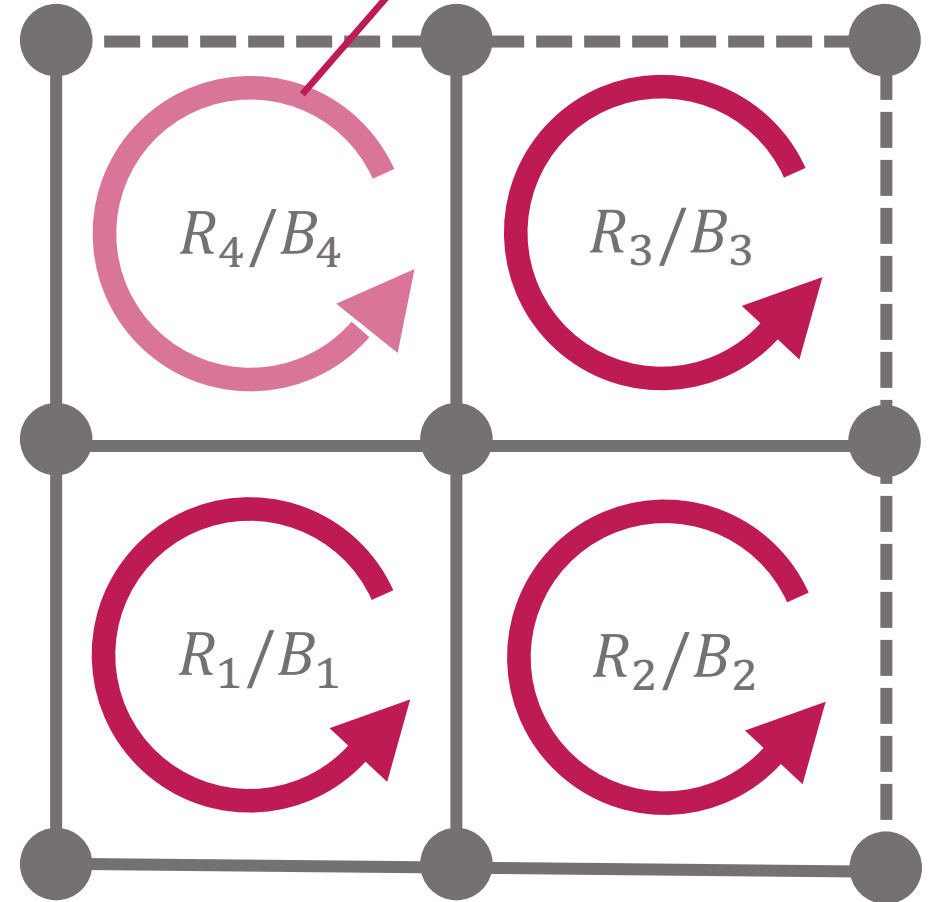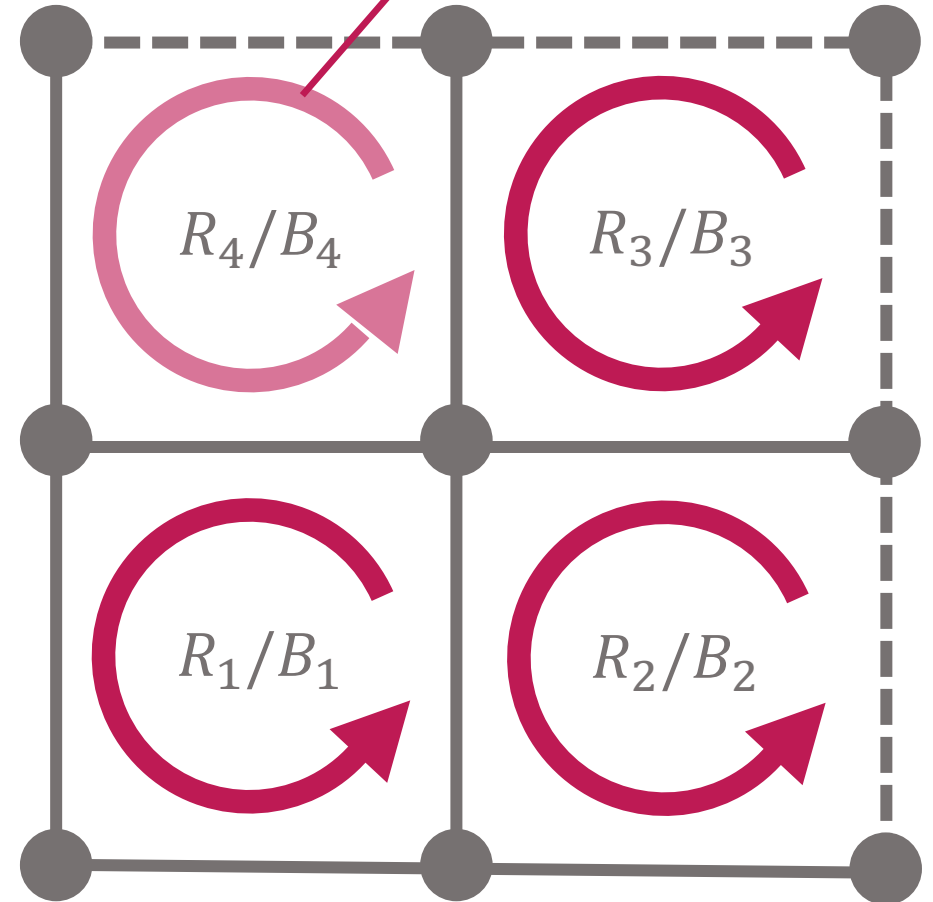
Pure compact U(1) LGT

- Eigenvalues of B fields are compactified $(-\pi, \pi]$

- R and B hold Canonical Commutation Relation (CCR):

$$[B_p, R_{p'}] = i\delta_{p,p'}$$

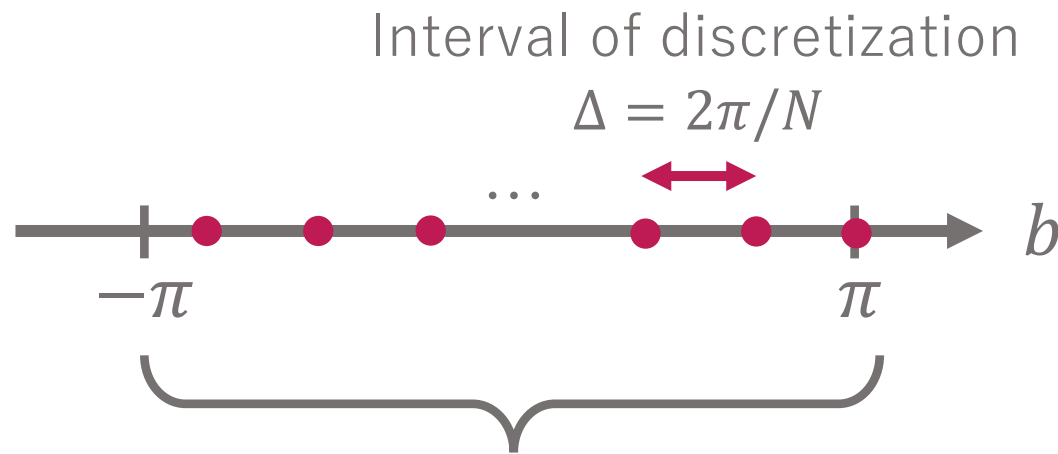- We take $a = 1$

R_4/B_4 can be removed by P.B.C.

Naive truncation method

- Consider representing those fields by finite dimensional matrices
- Naively, we can discretize those fields by equidistant points:

$$B = \int_{-\pi}^{\pi} db\, b|b\rangle\langle b| \rightarrow \tilde{B} = \sum_j b_j\, |b_j\rangle\langle b_j|,$$

$$b_j = j\frac{2\pi}{N}\ (j = -\lfloor N\rfloor/2, \ldots, \lfloor N\rfloor/2)$$

N: Discretization points

Interval of discretization

$$\Delta = 2\pi/N$$

$$\ldots$$

b

$-\pi$　　　　　π

Divide field values with N equidistant points

- N is related to number of qubits to do simulation
- By $N \rightarrow \infty$, theory after truncation returns to original theory

Naive truncation method

- Consider representing those fields by finite dimensional matrices
- Naively, we can discretize those fields by equidistant points:

$$B = \int_{-\pi}^{\pi} db \, b|b\rangle\langle b| \rightarrow \tilde{B} = \sum_{j} b_j \, |b_j\rangle\langle b_j|, \qquad b_j = j\frac{2\pi}{N} \ (j = -\lfloor N \rfloor/2, \dots, \lfloor N \rfloor/2)$$

- By discrete Fourier transformation, R is given by

$$R = \sum_{m=-\infty}^{\infty} r_m|r_m\rangle\langle r_m| \rightarrow \tilde{R} = \sum_{m=-\lfloor N \rfloor/2}^{\lfloor N \rfloor/2} r_m|r_m\rangle\langle r_m|$$

$$= \sum_{m=-\lfloor N \rfloor/2}^{\lfloor N \rfloor/2} m(\frac{1}{\sqrt{N}}\sum_{j} e^{i\frac{2\pi}{N}jm} \, |b_j\rangle)(\frac{1}{\sqrt{N}}\sum_{k} e^{-i\frac{2\pi}{N}km} \, \langle b_k|)$$

Canonical Commutation Relation method

CCR method [C. W. Bauer, D. M. Grabowska, 2023]

- CCR method is the method which optimize interval of gauge fields Δ
- We define loss function regarding CCR violation of ground states:

$$L(\Delta) \equiv \sum_{p \in \wp} |\langle \Psi_{\text{G.S.}}|[\tilde{B}_p, \tilde{R}_p] - i|\Psi_{\text{G.S.}}\rangle|$$
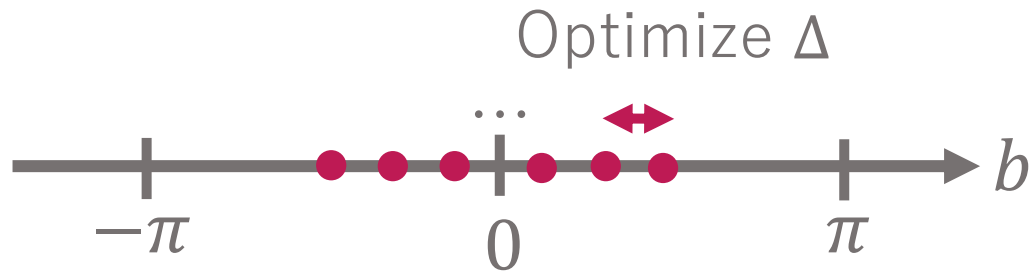
$\tilde{B}_p/\tilde{R}_p$: Magnetic/Rotator operator after discretization at each plaquette
$|\Psi_{\text{G.S.}}\rangle$: Ground state obtained by diagonalizing discretized Hamiltonian
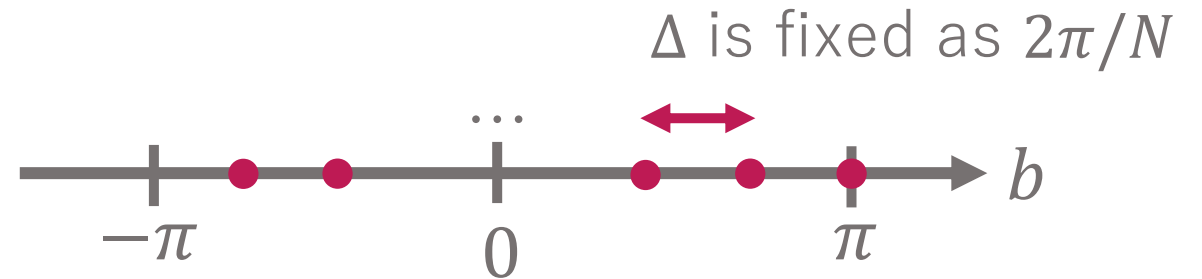
- We obtain Δ to minimize this loss function:

$$\Delta^* = \underset{\Delta}{\text{argmin}}\, L(\Delta)$$

Comparison of both methods

【CCR method】

【Naive truncation method】

Optimize Δ

Δ is fixed as $2\pi/N$

$-\pi$ 0 π b

$-\pi$ 0 π b

- CCR method can represent sharp wavefunction better than naive truncation method

- When $g \to 0$, contribution of magnetic Hamiltonian becomes dominant

▶ Wavefunction becomes sharper with small g

▶ Anticipated that CCR method is effective in the region of small g

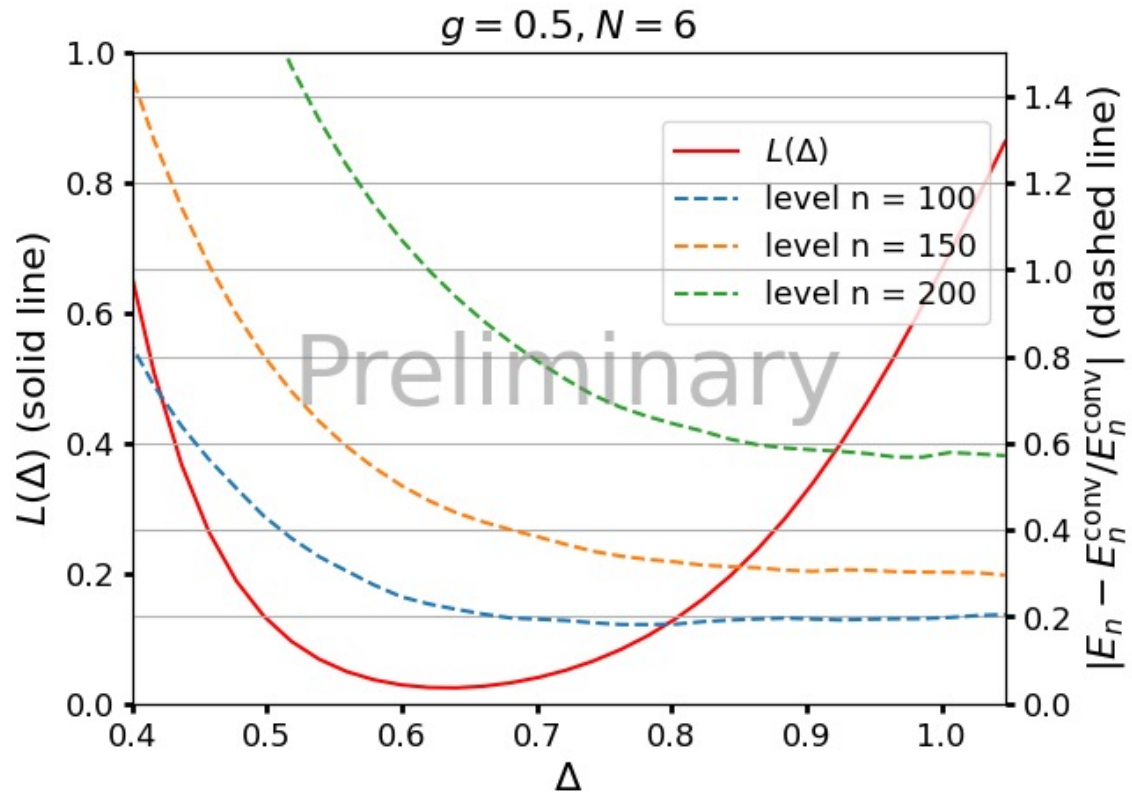# Loss function and errors of energy spectrums

【Low-lying levels】
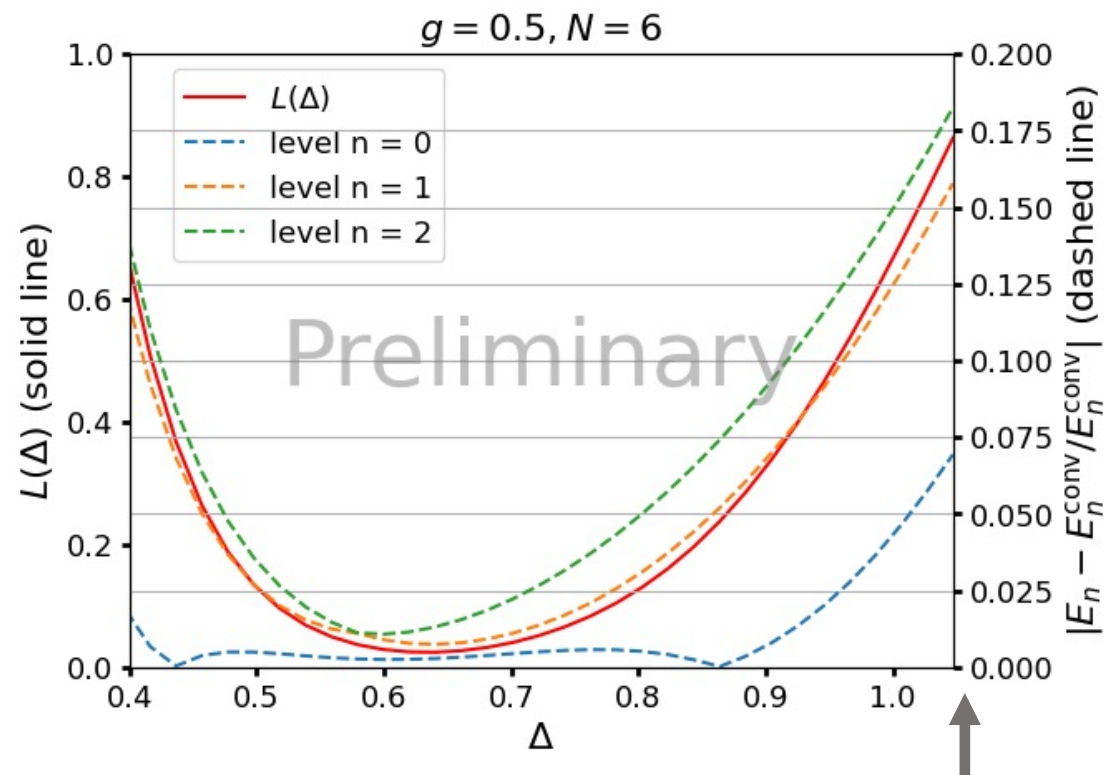
- In low-lying levels, CCR method optimize energy spectrums (consist with previous work)

E_n: Numerical values by CCR method with $N = 6$
E_n^{conv}: Converged values by Naive truncation method with large N

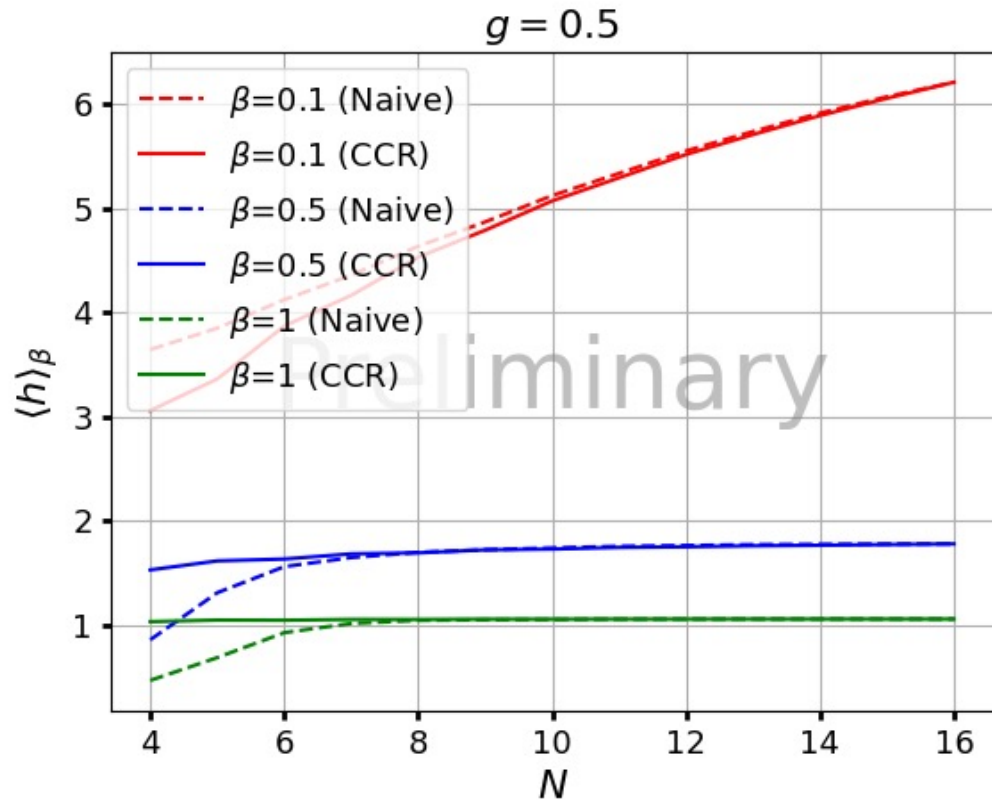This Δ is equivalent with Naive truncation method

Loss function and error of energy spectrums

【Excited levels】

$g = 0.5, N = 6$

Legend:
- $L(\Delta)$
- level n = 100
- level n = 150
- level n = 200

y-axis (left): $L(\Delta)$ (solid line)
y-axis (right): $|E_n - E_n^{conv}/E_n^{conv}|$ (dashed line)
x-axis: Δ

Preliminary

- In excited levels, optimized Δ moves to larger values

- Excited states becomes more spread out
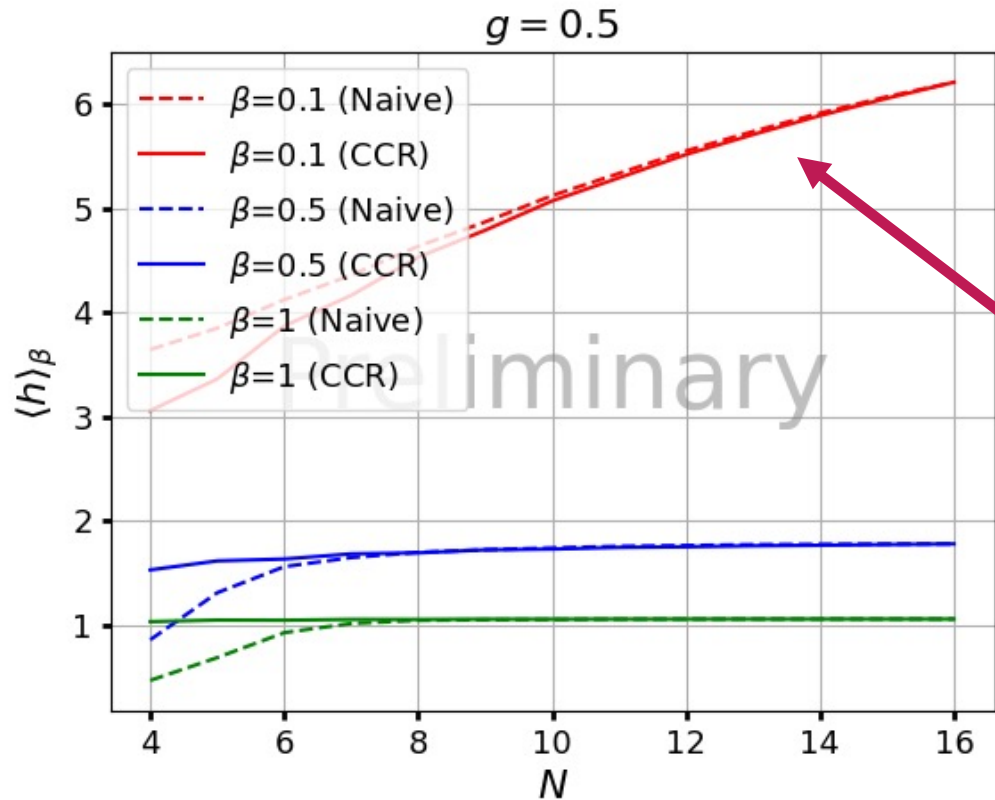
▶ Need to take gauge fields in wider range

Thermal observables

$g = 0.5$

Legend:
- $\beta = 0.1$ (Naive) — red dashed
- $\beta = 0.1$ (CCR) — red solid
- $\beta = 0.5$ (Naive) — blue dashed
- $\beta = 0.5$ (CCR) — blue solid
- $\beta = 1$ (Naive) — green dashed
- $\beta = 1$ (CCR) — green solid

- As a benchmark for calculation of thermal observables, we compute thermal expectation value of energy density:

$$\langle h \rangle_\beta := \mathrm{tr}(He^{-\beta H})/V$$

Thermal observables

$g = 0.5$

Legend:
- $\beta=0.1$ (Naive)
- $\beta=0.1$ (CCR)
- $\beta=0.5$ (Naive)
- $\beta=0.5$ (CCR)
- $\beta=1$ (Naive)
- $\beta=1$ (CCR)

Preliminary

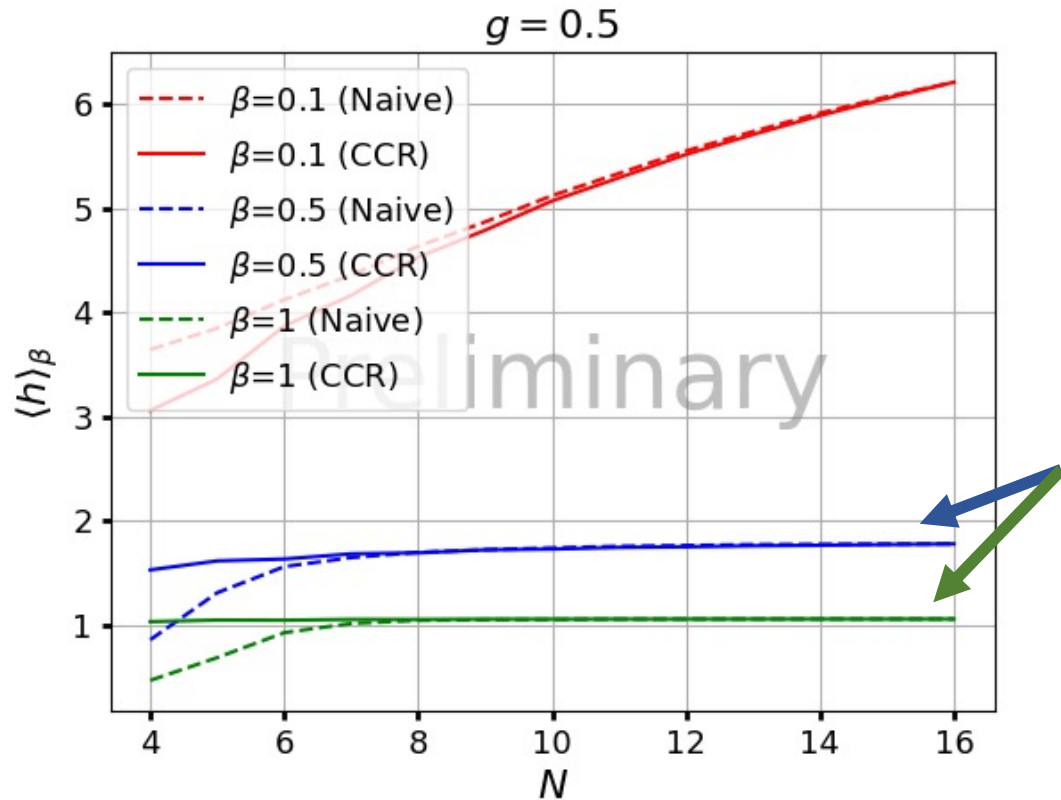- As a benchmark for calculation of thermal observables, we compute thermal expectation value of energy density:

$$\langle h \rangle_\beta := \mathrm{tr}(H e^{-\beta H})/V$$

High temperature region
- Both methods did not converge
- Contribution of excited states becomes dominant
▶ Figure indicates that both truncation is insufficient to represent quantum states

Thermal observables

$g = 0.5$

Legend:
- $\beta=0.1$ (Naive) — red dashed
- $\beta=0.1$ (CCR) — red solid
- $\beta=0.5$ (Naive) — blue dashed
- $\beta=0.5$ (CCR) — blue solid
- $\beta=1$ (Naive) — green dashed
- $\beta=1$ (CCR) — green solid

■ As a benchmark for calculation of thermal observables, we compute thermal expectation value of energy density:

$$\langle h \rangle_\beta := \operatorname{tr}(H e^{-\beta H})/V$$

Low temperature region

■ CCR method shows better convergence compared with naive truncation method

■ Indicates that we can simulate gauge fields with less qubits

Compact U(1) LGT including fermion

■ Hamiltonian:

$$H = H_E^{\text{(matter)}} + H_B + H_K + H_M$$

Mass term of fermion

Electric Hamiltonian is modified by the change of Gauss' law:
$$(\nabla \cdot \boldsymbol{E_n} - q_n)|\text{phys}\rangle = 0$$

Compact U(1) LGT including fermion

- Hamiltonian:

$$H = H_E^{(\mathbf{matter})} + H_B + \underline{H_K} + H_M$$
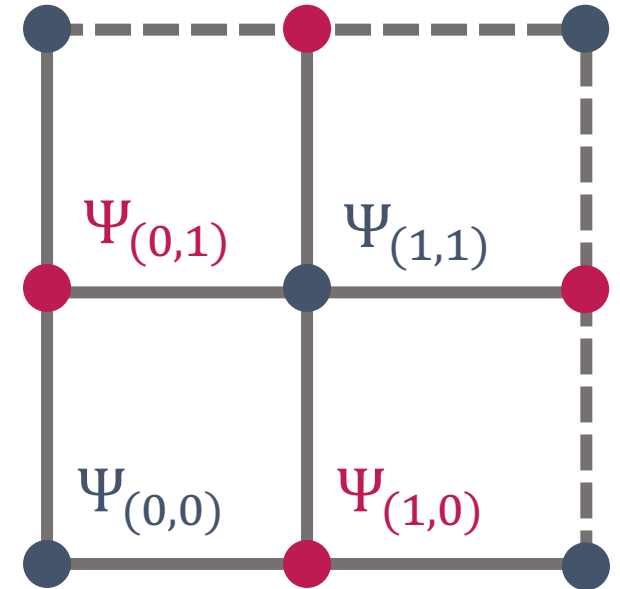
Interaction between
gauge fields and fermion

Compact U(1) LGT including fermion

- Hamiltonian:

$$H = H_E^{(\text{matter})} + H_B + H_K + H_M$$

- We take staggered fermion

$$\{\Psi_n^\dagger, \Psi_{n'}\} = \delta_{n,n'}$$

$\Psi_{(0,1)}$ $\Psi_{(1,1)}$

$\Psi_{(0,0)}$ $\Psi_{(1,0)}$

● : Matter
● : Anti matter

Compact U(1) LGT including fermion

- Hamiltonian:

$$H = H_E^{(\text{matter})} + H_B + H_K + H_M$$

- We take staggered fermion
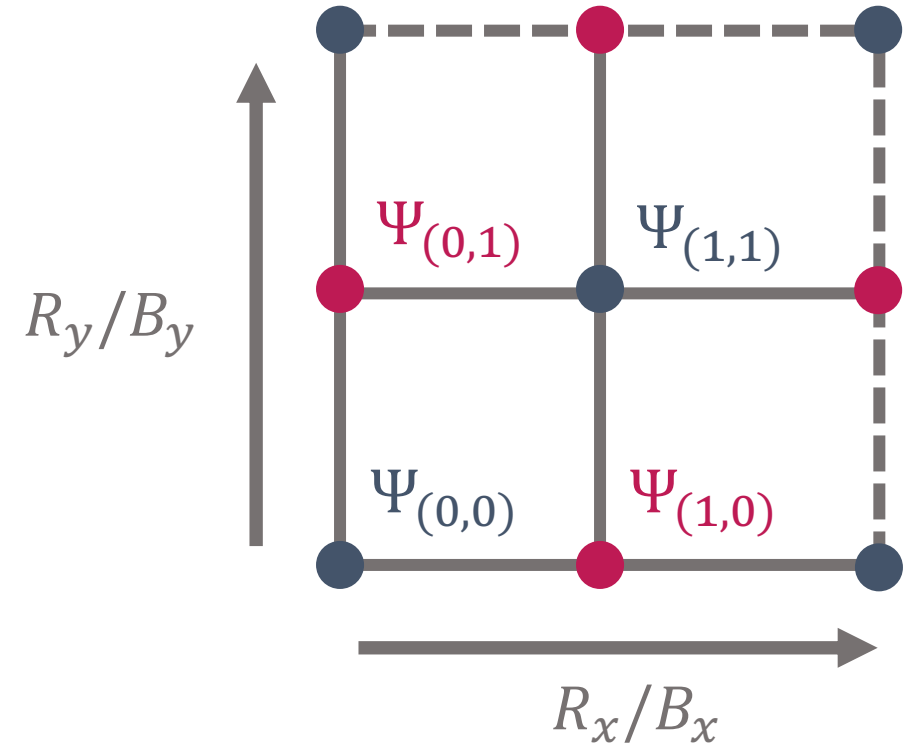
$$\{\Psi_n^\dagger, \Psi_{n'}\} = \delta_{n,n'}$$

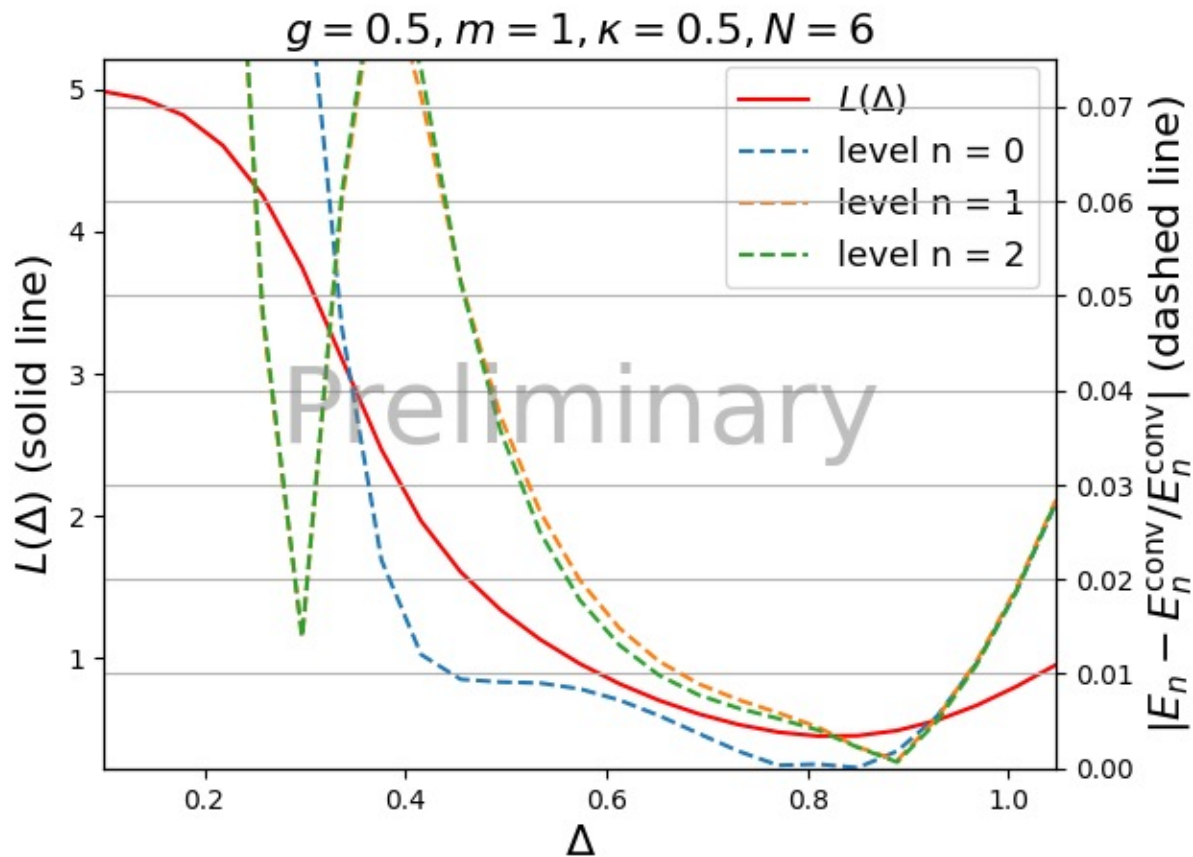- In addition to fermion, we need to consider
  - string operators: $R_{x/y}$
  - conjugate of string fields: $B_{x/y}$

- They also satisfy CCR: $[B_\mu, R_\nu] = i\delta_{\mu,\nu}$ ($\mu, \nu = 1, 2, 3, x, y$)

R_y/B_y

$\Psi_{(0,1)}$ $\Psi_{(1,1)}$

$\Psi_{(0,0)}$ $\Psi_{(1,0)}$

R_x/B_x

● : Matter
● : Anti matter

Loss function and errors of energy spectrums

$g = 0.5, m = 1, \kappa = 0.5, N = 6$

Preliminary

- Extend loss function to optimize string operators:

$$L(\Delta) \equiv \sum_{i=1,2,3,x,y} |\langle\Psi_{\text{G.S.}}|[\tilde{B}_i, \tilde{R}_i] - i|\Psi_{\text{G.S.}}\rangle|$$

- In this parameter, CCR method optimize low-lying states

m: Coefficient of H_M
κ: Coefficient of H_K

Thermal expectation value of energy density

$g = 0.5, m = 1, \kappa = 0.5$

Preliminary

Legend:
- $\beta = 3.0$ (Naive)
- $\beta = 3.0$ (CCR)
- $\beta = 10.0$ (Naive)
- $\beta = 10.0$ (CCR)

Axes: $\langle h \rangle_\beta$ vs N
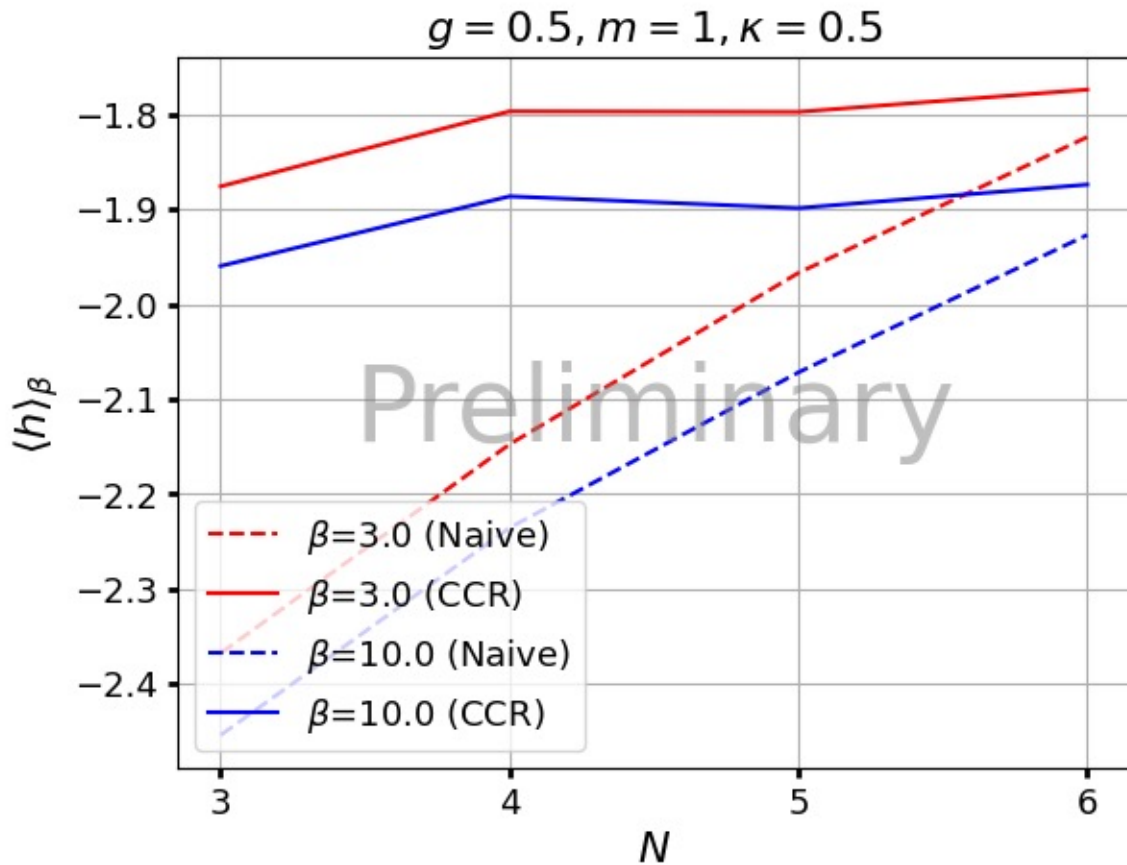
- CCR method shows better convergence than naive truncation method regarding with $\langle h \rangle_\beta$

- Indicates that CCR methods tell better representation of quantum states under $T \neq 0$

Conclusion

Summary

- In both theories, CCR method shows better convergence about thermal observables than naive truncation method

Future direction

- Extend to larger systems

- Extend to non-abelian theory

- Implement quantum algorithms ▶ Observe physical quantities

Appendix

Why do we consider (2+1)-dimensional theory?

- In (2+1)-dimensional LGT, D.O.F. of gauge fields remains even solving Gauss' law (constraints)

▶ Important to consider contributions of gauge fields seriously!

- In (1+1)-dimensional LGT, we can solve gauge fields D.O.F. completely under periodic boundary condition
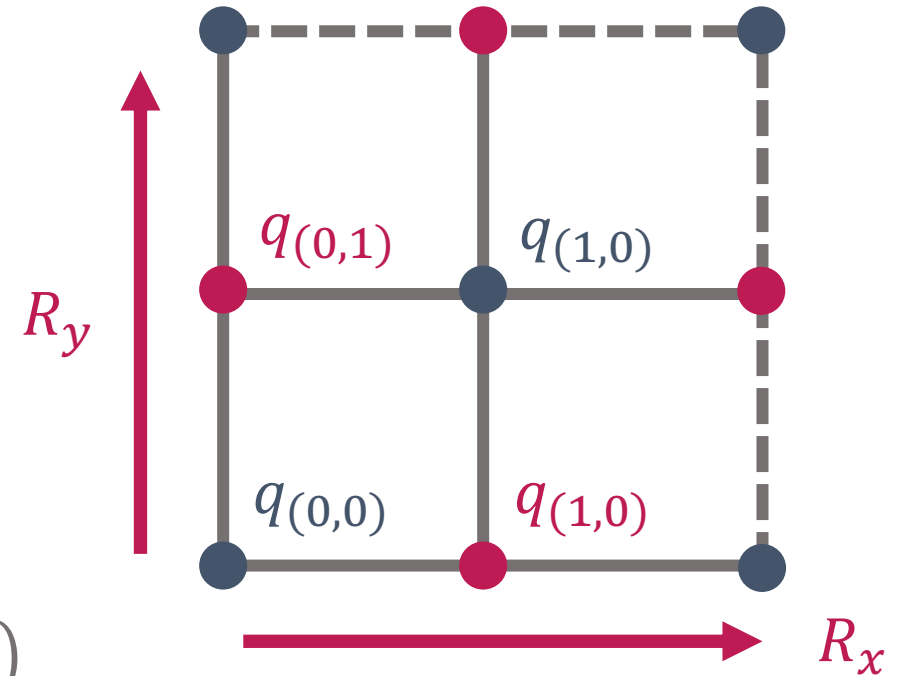
Details of $H_E^{(matter)}$

- Hamiltonian：

$$H = H_E^{(\text{matter})} + H_B^{(\text{C.})} + H_K + H_M$$

Electric Hamiltonian have interactions between rotator, string and fermion：

$$
\begin{aligned}
aH_E^{(\text{matter})} = g^2 \{ &2[R_1^2 + R_2^2 + R_3^2 - R_1(R_1 + R_3)] \\
&+ R_x^2 + R_y^2 + (R_1 + R_2 - R_3)R_x \\
&- (R_1 - R_2 - R_3)R_y \\
&- [q_{(1,0)}(R_1 + R_x) + q_{(0,1)}(R_2 - R_1 + R_y) \\
&+ q_{(1,1)}(2R_1 - R_2 + R_x)] \\
&+ \frac{q_{(1,0)}^2 + q_{(0,1)}^2 + 2q_{(1,1)}(q_{(1,0)} + q_{(1,1)})}{2} \}
\end{aligned}
$$

$R_{x/y}$：string operator
q_n：charge operator at site n

Details of H_K
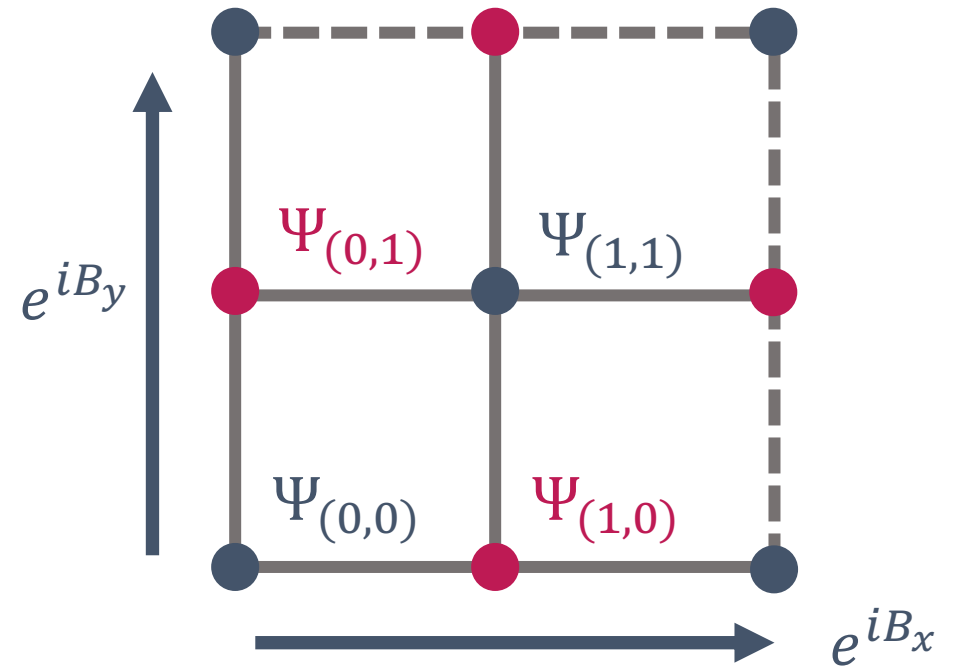
- Hamiltonian :

$$H = H_E^{(\text{matter})} + H_B + H_K + H_M$$

Interaction :

$$aH_K = \kappa \,[\Psi_{(0,0)}^{\dagger}\left(1 + e^{iB_x}\right)\Psi_{(1,0)}$$

$$+\Psi_{(0,1)}^{\dagger}\left(e^{iB_1} + e^{-iB_2}e^{iB_x}\right)\Psi_{(1,1)}$$

$$+\Psi_{(0,0)}^{\dagger}\left(1 + e^{iB_y}\right)\Psi_{(0,1)}$$

$$+\Psi_{(1,0)}^{\dagger}\left(1 + e^{-iB_2}e^{-iB_3}e^{iB_y}\right)\Psi_{(1,1)} + \text{H.c.}\,]$$

$$\kappa = 1/2$$

Details of H_B and H_M

- Hamiltonian：

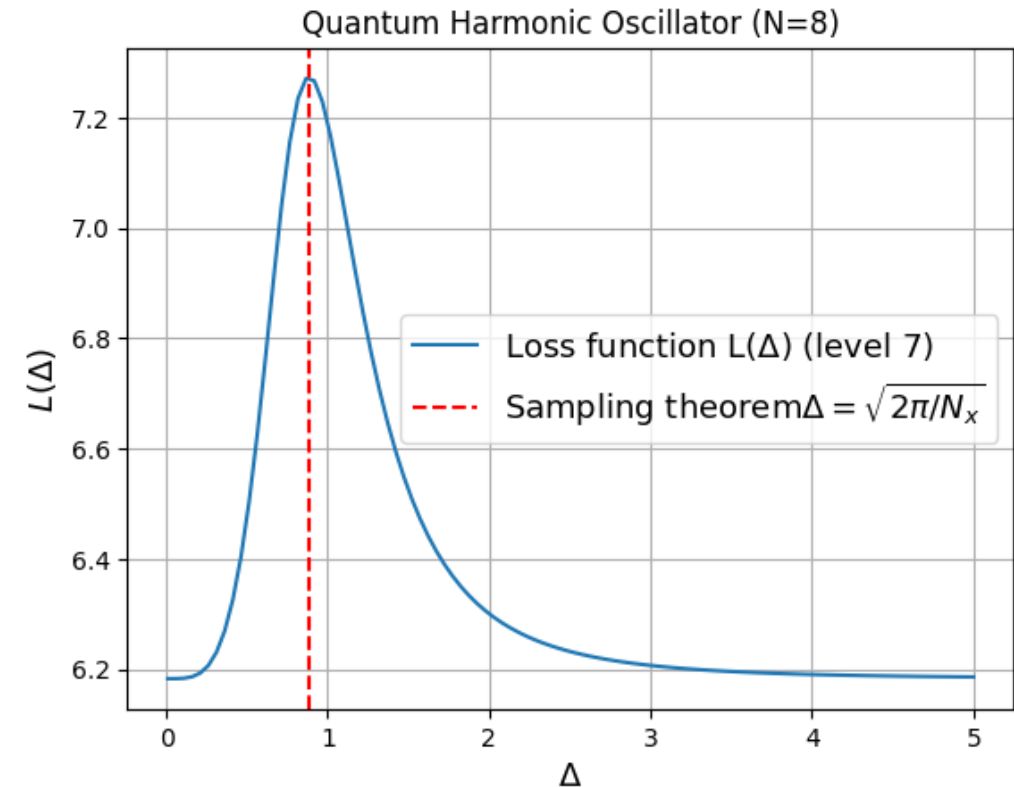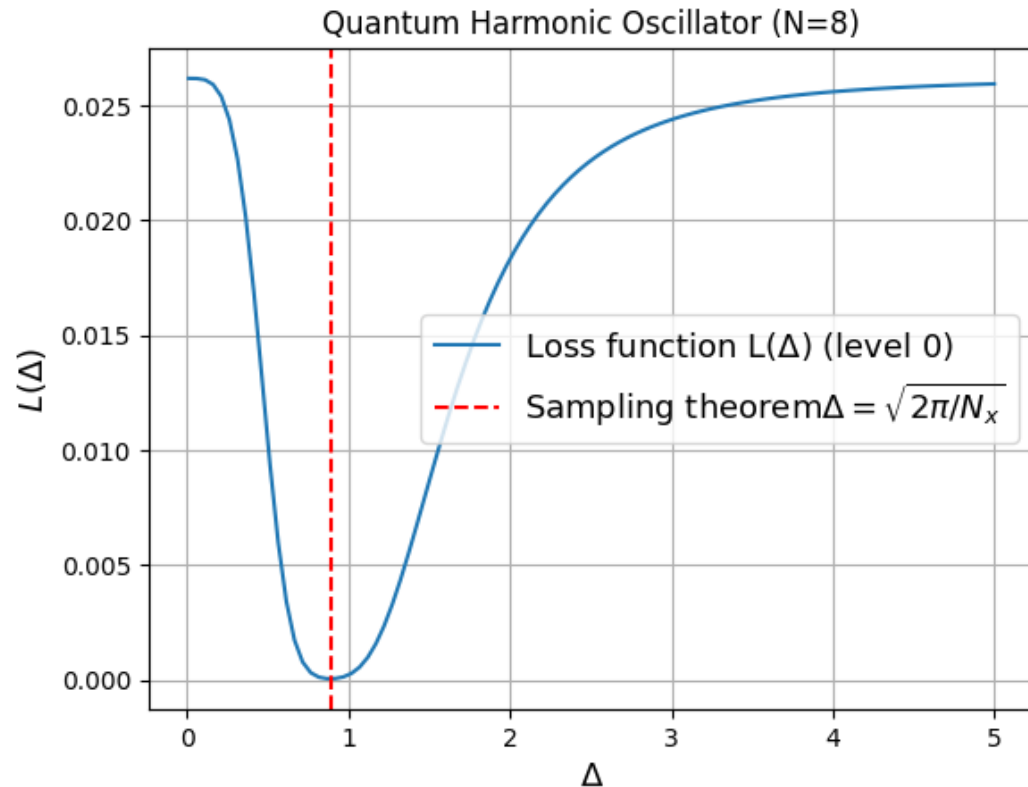$$H = H_E^{(\text{matter})} + H_B^{(\text{C.})} + H_K + H_M$$

Magnetic Hamiltonian：

$$aH_B^{(\text{C.})} = -\frac{1}{g^2}[\cos(B_1) + \cos(B_2) + \cos(B_3)$$
$$+\cos(B_1 + B_2 + B_3)]$$
$$\propto \mathcal{O}(1/g^2)$$

Mass term：

$$aH_M = m[\Psi_{(0,0)}^{\dagger}\Psi_{(0,0)} - \Psi_{(0,1)}^{\dagger}\Psi_{(0,1)}$$
$$+\Psi_{(1,1)}^{\dagger}\Psi_{(1,1)} - \Psi_{(1,0)}^{\dagger}\Psi_{(1,0)}]$$
$$\propto \mathcal{O}(m)$$

Why do we compute expectation values with ground states?

- Numerical computations in Quantum Harmonic Oscillator indicate that we cannot optimize adequately by taking expectation values with excited states

Loss function

- Eigenvalues of magnetic operators are compactified $(-\pi, \pi]$
▶ Possibility that range of magnetic fields goes beyond 2π after optimization
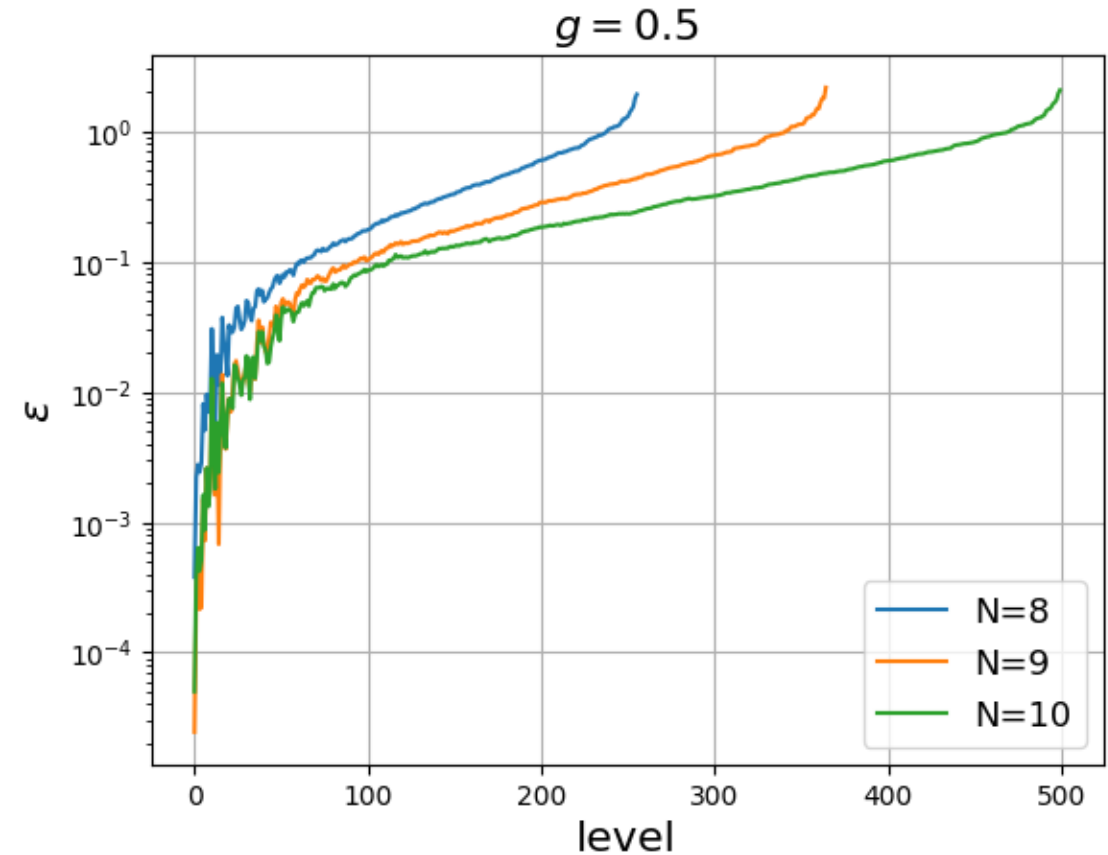▶ In this case, we respect the 2π range of magnetic fields, that is,

$$\Delta = \min\{\Delta^*, 2\pi/N\}$$

$\Delta^* : \Delta$ obtained by optimizing $L(\Delta)$

※In the case of $\Delta = 2\pi/N$, discretized Hamiltonian by CCR method becomes equivalent with truncated KS method

Error at each level in pure compact U(1) LGT

- Error at each level in pure compact U(1) LGT by CCR method

- Errors increase exponentially
  with increase of levels

Check convergence of $E_n^{\mathbf{conv}}$

- $E_n^{(N)}$: Energy spectrums obtained by Exact Diagonalization of

    Hamiltonian after discretization with N discretization points

- Define "convergence of $E_n^{(N)}$ with precision δ" as differences between energy spectrums with $N-1$ and with N is smaller than δ, that is,

$$\left| \frac{E_n^{(N-1)} - E_n^{(N)}}{E_n^{(N)}} \right| < \delta$$

- We take $\delta = 10^{-3}$

Calculation of thermal observables in compact U(1) with fermion

- Difficult to compute all eigenvalues due to huge size of matrices

- We compute $\langle h \rangle_\beta^{(N_{\text{cutoff}})}$:

$$\langle h \rangle_\beta^{(N_{\text{cutoff}})} = \frac{1}{V} \frac{\sum_{n=0}^{N_{\text{cutoff}}-1} E_n e^{-\beta E_n}}{\sum_{n=0}^{N_{\text{cutoff}}-1} e^{-\beta E_n}}$$

  where N_{cutoff} is cutoff level

- We regard $\langle h \rangle_\beta^{(N_{\text{cutoff}})}$ to $\langle h \rangle_\beta$ with precision δ if

$$\left| \frac{\langle h \rangle_\beta^{(N_{\text{cutoff}}-1)} - \langle h \rangle_\beta^{(N_{\text{cutoff}})}}{\langle h \rangle_\beta^{(N_{\text{cutoff}})}} \right| < \delta$$

- We take $\delta = 10^{-3}$